Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 3-(3-Methylphenyl)-5-(quinolin-8-ylmethoxy)-1,2,4-oxadiazole monohydrate

**Lu Yang,[a,b] Wei Liu,[a,b] Han Wang,[a,b]* Xing-Wei Chen[a,b] and Hai-Bo Wang[b]**

[a]College of Science, Nanjing University of Technology, Xinmofan Road No.5 Nanjing, Nanjing 210009, People's Republic of China, and [b]College of Food Science and Light Industry, Nanjing University of Technology, Xinmofan Road No.5 Nanjing, Nanjing 210009, People's Republic of China
Correspondence e-mail: wanghaibo@njut.edu.cn

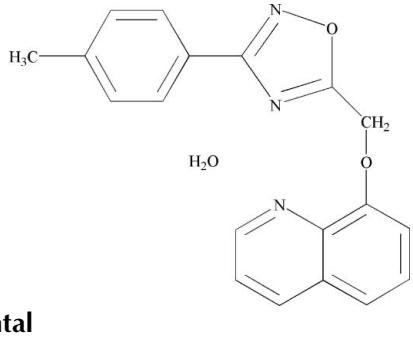
Received 3 April 2013; accepted 5 September 2013

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.054; $wR$ factor = 0.162; data-to-parameter ratio = 13.0.

In the title compound, $C_{19}H_{15}N_3O_2\cdot H_2O$, the oxadiazole ring and the quinoline unit are almost coplanar, making a dihedral angle of 7.66 (8)°. The dihedral angle between the benzene ring and the quinoline system is 25.95 (8)° while that between the benzene and the oxadiazole rings is 18.88 (9)°. The water molecule is hydrogen bonded to an oxadiazole N atom and to the quinoline N atom. In the crystal, these units are linked *via* C—H···O hydrogen bonds, forming two-dimensional networks lying parallel to the *ab* plane.

## Related literature

For the preparation of the title compound, see: Chiou & Shine (1989). For the biological activity of 1,2,4-oxadiazole derivatives, see: Street *et al.* (1990). For metal complexes of related compounds, see: da Silva *et al.* (1999); Pibiri *et al.* (2010); Terenzi *et al.* (2011). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{19}H_{15}N_3O_2\cdot H_2O$
$M_r$ = 335.36
Triclinic, $P\overline{1}$
$a$ = 7.2070 (14) Å
$b$ = 7.6200 (15) Å
$c$ = 15.109 (3) Å
$\alpha$ = 92.62 (3)°
$\beta$ = 90.19 (3)°
$\gamma$ = 92.15 (3)°
$V$ = 828.3 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.30 × 0.10 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.973, $T_{max}$ = 0.991
3302 measured reflections
3039 independent reflections
1949 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.015
3 standard reflections every 200 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.162
$S$ = 1.00
3039 reflections
233 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| $OW$—H$WB$···N2 | 0.91 (3) | 2.09 (3) | 2.980 (3) | 169 (3) |
| $OW$—H$WA$···N1 | 0.94 (3) | 1.91 (3) | 2.830 (3) | 165 (3) |
| C7—H7$A$···$OW^{i}$ | 0.93 | 2.51 | 3.272 (3) | 139 |
| C10—H10$A$···$OW^{ii}$ | 0.97 | 2.55 | 3.482 (3) | 160 |
| C10—H10$B$···$OW^{iii}$ | 0.97 | 2.59 | 3.534 (3) | 164 |

Symmetry codes: (i) $-x-1, -y+1, -z+2$; (ii) $x+1, y, z$; (iii) $-x, -y+2, -z+2$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2428).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Chiou, S. & Shine, H. J. (1989). *J. Heterocycl. Chem.* **26**, 125–128.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Pibiri, I., Piccionello, A. P., Calabrese, A., Buscemi, S., Vivona, N. & Pace, A. (2010). *Eur. J. Org. Chem.* pp. 4549–4553.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Silva, A. S. da, de Silva, M. A. A., Carvalho, C. E. M., Antunes, O. A. C., Herrera, J. O. M., Brinn, I. M. & Mangrich, A. S. (1999). *Inorg. Chim. Acta* **292**, 1–6.
Street, L. J., Baker, R., Book, T., Kneen, C. O., MacLeod, A. M., Merchant, K. J., Showell, G. A., Saunders, J., Herbert, R. H., Freedman, S. B. & Harley, E. A. (1990). *J. Med. Chem.* **33**, 2690–2697.
Terenzi, A., Barone, G., Piccionello, A. P., Giorgi, G., Guarecello, A. & Pace, A. (2011). *Inorg. Chim. Acta*, **373**, 62–67.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supplementary materials

*Acta Cryst.* (2013). E**69**, o1541 [doi:10.1107/S160053681302477X]

## 3-(3-Methylphenyl)-5-(quinolin-8-ylmethoxy)-1,2,4-oxadiazole monohydrate

**Lu Yang, Wei Liu, Han Wang, Xing-Wei Chen and Hai-Bo Wang**

### 1. Comment

1,2,4-Oxadiazole derivatives have shown high biological activity, such as antibacterial, anti-HIV and weed control (Street *et al.*, 1990). They are therefore widely used in medicinal chemistry and as pesticides. 1,2,4-Oxadiazole derivatives in combination with metal ions can also be used in fluorescent recognition (da Silva *et al.*, 1999; Pibiri *et al.*, 2010; Terenzi *et al.*, 2011). The title compound 5-(quinoline-8-ylmethoxy)-3-p-tolyl-1,2,4-oxadiazole was also used in metal ions fluorescent recognition. In the molecule of 5-(quinoline-8-ylmethoxy)-3-p-tolyl-1,2,4-oxadiazole hydrate (Fig. 1) bond lengths (Allen *et al.*, 1987) and angles are within normal ranges.The oxadiazol ring and the quinoline moiety are almost coplanar showing a dihedral angle of 7.66 (8)°. The dihedral angles between the benzene ring and the quinoline system is 25.95 (8)°, the corresponding angle between the benzene and the oxadiazol rings is 18.88 (9)°. The crystal structure is established by intermolecular N—H···O and O—H···O hydrogen bonds (Fig. 2).

### 2. Experimental

5-(Quinoline-8-ylmethoxy)-3-p-tolyl-1,2,4-oxadiazole was prepared by a literature method (Chiou & Shine, 1989). 3-(4-Methyl-phenyl)-5-chloromethyl-1,2,4-oxadizole (3.4 g, 16.4 mmol), 8-hydroxy-quinoline (2.4 g, 16.4 mmol), potassium carbonate (3.4 g ,24.6 mmol) and potassium iodide (catalytic amount) were added to acetone (40 ml). The mixture was then heated to reflux for 6 hours. After being cooled to room temperature, the mixture was filtered and evaporated to afford the product as a yellow solid. The crude product was re-crystallized from ethyl acetate (yield 3.1g, 59.8%). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate solution.

### 3. Refinement

H atoms were positioned geometrically, with C-H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,N)$, where x = 1.5 for methyl H and x = 1.2 for all other H atoms. Hydrogen atoms of the solvent water molecule have been determined from Fourier maps and refined freely.

### Computing details

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *publCIF* (Westrip, 2010).

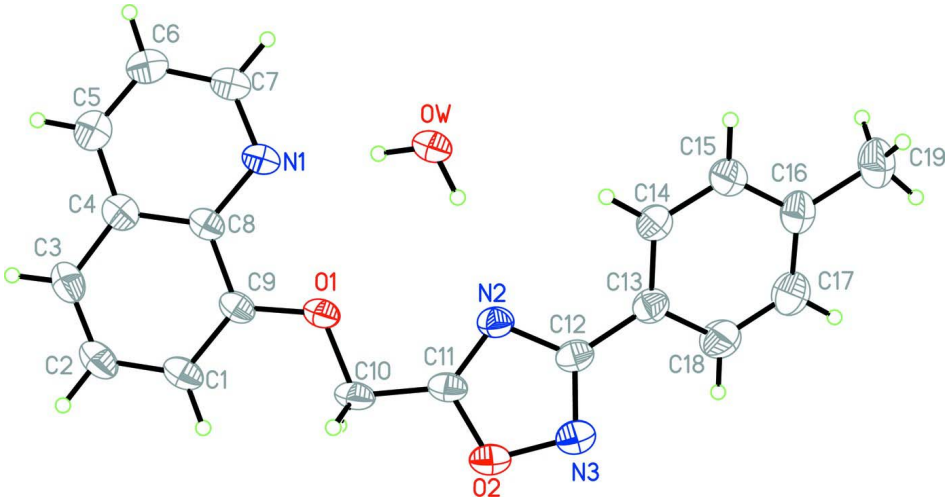



**Figure 1**

Molecular structure of the title molecule with displacement ellipsoids drawn at the 50% probability level.

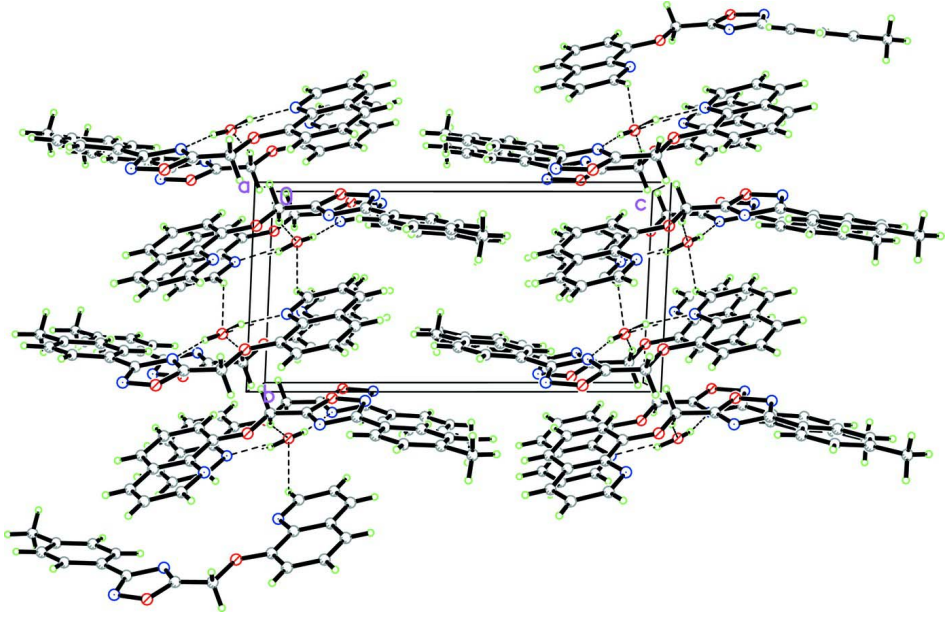


**Figure 2**

Packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

### 3-(3-Methylphenyl)-5-(quinolin-8-ylmethoxy)-1,2,4-oxadiazole monohydrate

*Crystal data*

$C_{19}H_{15}N_3O_2 \cdot H_2O$
$M_r = 335.36$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2070\ (14)$ Å
$b = 7.6200\ (15)$ Å
$c = 15.109\ (3)$ Å
$\alpha = 92.62\ (3)°$
$\beta = 90.19\ (3)°$
$\gamma = 92.15\ (3)°$
$V = 828.3\ (3)$ Å$^3$
$Z = 2$
$F(000) = 352$
$D_x = 1.345$ Mg m$^{-3}$
Melting point: 342 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–13°$

$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K

Block, yellow
0.30 × 0.10 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.973, $T_{max}$ = 0.991
3302 measured reflections

3039 independent reflections
1949 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.015
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 1.4°
$h$ = 0→8
$k$ = −9→9
$l$ = −18→18
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.162
$S$ = 1.00
3039 reflections
233 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.097P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.033 (7)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.0819 (2) | 0.7951 (2) | 0.99656 (11) | 0.0571 (5) |
| N1 | −0.1889 (3) | 0.6301 (2) | 1.08273 (13) | 0.0522 (5) |
| C1 | 0.2813 (3) | 0.8077 (3) | 1.12657 (18) | 0.0596 (7) |
| H1B | 0.3763 | 0.8670 | 1.0974 | 0.071* |
| N2 | 0.0057 (3) | 0.8438 (2) | 0.81930 (13) | 0.0511 (5) |
| O2 | 0.2873 (2) | 0.9553 (2) | 0.80096 (12) | 0.0695 (6) |
| C2 | 0.3046 (4) | 0.7675 (4) | 1.21478 (19) | 0.0667 (7) |
| H2B | 0.4155 | 0.8005 | 1.2437 | 0.080* |
| C3 | 0.1700 (4) | 0.6819 (4) | 1.25913 (18) | 0.0656 (7) |
| H3A | 0.1894 | 0.6553 | 1.3178 | 0.079* |
| N3 | 0.2016 (3) | 0.9460 (3) | 0.71676 (15) | 0.0714 (7) |
| C4 | −0.0008 (3) | 0.6320 (3) | 1.21701 (17) | 0.0551 (6) |

| | | | | |
|---|---|---|---|---|
| C5 | −0.1489 (4) | 0.5465 (3) | 1.25918 (18) | 0.0642 (7) |
| H5A | −0.1374 | 0.5179 | 1.3181 | 0.077* |
| C6 | −0.3092 (4) | 0.5051 (3) | 1.21418 (19) | 0.0653 (7) |
| H6A | −0.4084 | 0.4483 | 1.2416 | 0.078* |
| C7 | −0.3218 (3) | 0.5497 (3) | 1.12629 (18) | 0.0594 (7) |
| H7A | −0.4323 | 0.5206 | 1.0962 | 0.071* |
| C8 | −0.0273 (3) | 0.6721 (3) | 1.12723 (16) | 0.0475 (6) |
| C9 | 0.1196 (3) | 0.7605 (3) | 1.08256 (16) | 0.0486 (6) |
| C10 | 0.2240 (3) | 0.8842 (3) | 0.94993 (17) | 0.0557 (6) |
| H10A | 0.3386 | 0.8219 | 0.9528 | 0.067* |
| H10B | 0.2460 | 1.0022 | 0.9757 | 0.067* |
| C11 | 0.1608 (3) | 0.8911 (3) | 0.85698 (17) | 0.0511 (6) |
| C12 | 0.0369 (3) | 0.8783 (3) | 0.73185 (16) | 0.0535 (6) |
| C13 | −0.0981 (3) | 0.8373 (3) | 0.66076 (16) | 0.0553 (6) |
| C14 | −0.2843 (4) | 0.8113 (3) | 0.67896 (17) | 0.0617 (7) |
| H14A | −0.3249 | 0.8161 | 0.7374 | 0.074* |
| C15 | −0.4105 (4) | 0.7784 (4) | 0.61087 (18) | 0.0687 (7) |
| H15A | −0.5356 | 0.7628 | 0.6245 | 0.082* |
| C16 | −0.3573 (4) | 0.7677 (3) | 0.52325 (17) | 0.0677 (8) |
| C17 | −0.1699 (5) | 0.7904 (4) | 0.50615 (19) | 0.0847 (9) |
| H17A | −0.1291 | 0.7826 | 0.4478 | 0.102* |
| C18 | −0.0424 (4) | 0.8242 (4) | 0.57307 (19) | 0.0814 (9) |
| H18A | 0.0828 | 0.8385 | 0.5594 | 0.098* |
| C19 | −0.4974 (5) | 0.7358 (4) | 0.45006 (19) | 0.0905 (10) |
| H19A | −0.4352 | 0.7339 | 0.3940 | 0.136* |
| H19B | −0.5845 | 0.8282 | 0.4523 | 0.136* |
| H19C | −0.5622 | 0.6250 | 0.4571 | 0.136* |
| OW | −0.3313 (2) | 0.7299 (3) | 0.91840 (14) | 0.0733 (6) |
| HWB | −0.236 (5) | 0.757 (4) | 0.8819 (19) | 0.088* |
| HWA | −0.274 (4) | 0.682 (4) | 0.967 (2) | 0.088* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0383 (8) | 0.0683 (11) | 0.0639 (11) | −0.0106 (8) | −0.0065 (8) | 0.0075 (8) |
| N1 | 0.0400 (10) | 0.0500 (11) | 0.0661 (13) | −0.0038 (9) | −0.0033 (10) | 0.0013 (9) |
| C1 | 0.0387 (13) | 0.0624 (16) | 0.0769 (19) | 0.0010 (11) | −0.0102 (12) | −0.0030 (13) |
| N2 | 0.0425 (11) | 0.0550 (12) | 0.0551 (12) | −0.0019 (9) | 0.0074 (9) | −0.0021 (9) |
| O2 | 0.0450 (10) | 0.0884 (13) | 0.0744 (13) | −0.0133 (9) | 0.0078 (9) | 0.0081 (10) |
| C2 | 0.0498 (15) | 0.0751 (18) | 0.0742 (19) | 0.0041 (13) | −0.0197 (14) | −0.0088 (14) |
| C3 | 0.0634 (17) | 0.0752 (18) | 0.0579 (16) | 0.0075 (14) | −0.0165 (14) | −0.0034 (13) |
| N3 | 0.0556 (13) | 0.0913 (17) | 0.0670 (15) | −0.0103 (12) | 0.0084 (12) | 0.0106 (12) |
| C4 | 0.0528 (14) | 0.0486 (13) | 0.0640 (16) | 0.0094 (11) | −0.0032 (12) | −0.0022 (11) |
| C5 | 0.0694 (18) | 0.0598 (16) | 0.0643 (17) | 0.0119 (14) | 0.0029 (14) | 0.0052 (13) |
| C6 | 0.0580 (16) | 0.0608 (16) | 0.0773 (19) | −0.0011 (13) | 0.0091 (14) | 0.0079 (14) |
| C7 | 0.0457 (14) | 0.0567 (15) | 0.0753 (18) | −0.0028 (12) | −0.0016 (13) | 0.0017 (13) |
| C8 | 0.0405 (12) | 0.0420 (12) | 0.0595 (15) | 0.0032 (10) | −0.0053 (11) | −0.0046 (10) |
| C9 | 0.0370 (12) | 0.0478 (13) | 0.0607 (15) | 0.0047 (10) | −0.0081 (11) | −0.0021 (11) |
| C10 | 0.0327 (11) | 0.0617 (15) | 0.0713 (17) | −0.0062 (11) | 0.0050 (11) | −0.0053 (12) |
| C11 | 0.0351 (12) | 0.0505 (13) | 0.0668 (16) | −0.0005 (10) | 0.0058 (11) | −0.0041 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.0478 (13) | 0.0534 (14) | 0.0592 (16) | 0.0016 (11) | 0.0118 (11) | 0.0019 (11) |
| C13 | 0.0573 (15) | 0.0544 (14) | 0.0540 (15) | 0.0009 (12) | 0.0074 (12) | 0.0002 (11) |
| C14 | 0.0577 (15) | 0.0757 (17) | 0.0516 (15) | 0.0001 (13) | 0.0060 (12) | 0.0021 (12) |
| C15 | 0.0590 (15) | 0.0846 (19) | 0.0623 (18) | −0.0007 (14) | −0.0003 (13) | 0.0034 (14) |
| C16 | 0.085 (2) | 0.0642 (17) | 0.0536 (17) | 0.0042 (15) | −0.0039 (14) | 0.0020 (13) |
| C17 | 0.090 (2) | 0.112 (3) | 0.0512 (17) | −0.0007 (19) | 0.0109 (16) | −0.0037 (16) |
| C18 | 0.0700 (18) | 0.111 (2) | 0.0616 (18) | −0.0049 (17) | 0.0182 (16) | −0.0037 (16) |
| C19 | 0.111 (3) | 0.100 (2) | 0.0606 (18) | 0.003 (2) | −0.0170 (18) | 0.0006 (17) |
| OW | 0.0446 (10) | 0.1012 (15) | 0.0735 (13) | −0.0152 (10) | −0.0081 (9) | 0.0147 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C9 | 1.366 (3) | C7—H7A | 0.9300 |
| O1—C10 | 1.415 (3) | C8—C9 | 1.422 (3) |
| N1—C7 | 1.313 (3) | C10—C11 | 1.479 (4) |
| N1—C8 | 1.363 (3) | C10—H10A | 0.9700 |
| C1—C9 | 1.368 (3) | C10—H10B | 0.9700 |
| C1—C2 | 1.392 (4) | C12—C13 | 1.462 (3) |
| C1—H1B | 0.9300 | C13—C14 | 1.380 (4) |
| N2—C11 | 1.285 (3) | C13—C18 | 1.386 (4) |
| N2—C12 | 1.376 (3) | C14—C15 | 1.379 (4) |
| O2—C11 | 1.340 (3) | C14—H14A | 0.9300 |
| O2—N3 | 1.410 (3) | C15—C16 | 1.379 (4) |
| C2—C3 | 1.346 (4) | C15—H15A | 0.9300 |
| C2—H2B | 0.9300 | C16—C17 | 1.381 (4) |
| C3—C4 | 1.415 (3) | C16—C19 | 1.501 (4) |
| C3—H3A | 0.9300 | C17—C18 | 1.373 (4) |
| N3—C12 | 1.301 (3) | C17—H17A | 0.9300 |
| C4—C5 | 1.400 (4) | C18—H18A | 0.9300 |
| C4—C8 | 1.418 (3) | C19—H19A | 0.9600 |
| C5—C6 | 1.358 (4) | C19—H19B | 0.9600 |
| C5—H5A | 0.9300 | C19—H19C | 0.9600 |
| C6—C7 | 1.389 (4) | OW—HWB | 0.91 (3) |
| C6—H6A | 0.9300 | OW—HWA | 0.94 (3) |
| | | | |
| C9—O1—C10 | 116.60 (18) | O1—C10—H10B | 110.3 |
| C7—N1—C8 | 117.4 (2) | C11—C10—H10B | 110.3 |
| C9—C1—C2 | 120.5 (2) | H10A—C10—H10B | 108.5 |
| C9—C1—H1B | 119.8 | N2—C11—O2 | 113.4 (2) |
| C2—C1—H1B | 119.8 | N2—C11—C10 | 131.4 (2) |
| C11—N2—C12 | 103.1 (2) | O2—C11—C10 | 115.16 (19) |
| C11—O2—N3 | 105.97 (17) | N3—C12—N2 | 114.0 (2) |
| C3—C2—C1 | 121.4 (2) | N3—C12—C13 | 122.2 (2) |
| C3—C2—H2B | 119.3 | N2—C12—C13 | 123.9 (2) |
| C1—C2—H2B | 119.3 | C14—C13—C18 | 118.2 (3) |
| C2—C3—C4 | 120.4 (3) | C14—C13—C12 | 121.0 (2) |
| C2—C3—H3A | 119.8 | C18—C13—C12 | 120.8 (2) |
| C4—C3—H3A | 119.8 | C15—C14—C13 | 120.2 (2) |
| C12—N3—O2 | 103.59 (19) | C15—C14—H14A | 119.9 |
| C5—C4—C3 | 123.8 (3) | C13—C14—H14A | 119.9 |

| | | | |
|---|---|---|---|
| C5—C4—C8 | 117.1 (2) | C14—C15—C16 | 122.2 (3) |
| C3—C4—C8 | 119.0 (2) | C14—C15—H15A | 118.9 |
| C6—C5—C4 | 120.1 (3) | C16—C15—H15A | 118.9 |
| C6—C5—H5A | 120.0 | C15—C16—C17 | 116.9 (3) |
| C4—C5—H5A | 120.0 | C15—C16—C19 | 121.3 (3) |
| C5—C6—C7 | 118.5 (3) | C17—C16—C19 | 121.8 (3) |
| C5—C6—H6A | 120.7 | C18—C17—C16 | 121.7 (3) |
| C7—C6—H6A | 120.7 | C18—C17—H17A | 119.2 |
| N1—C7—C6 | 124.6 (2) | C16—C17—H17A | 119.2 |
| N1—C7—H7A | 117.7 | C17—C18—C13 | 120.8 (3) |
| C6—C7—H7A | 117.7 | C17—C18—H18A | 119.6 |
| N1—C8—C4 | 122.3 (2) | C13—C18—H18A | 119.6 |
| N1—C8—C9 | 119.1 (2) | C16—C19—H19A | 109.5 |
| C4—C8—C9 | 118.7 (2) | C16—C19—H19B | 109.5 |
| O1—C9—C1 | 125.1 (2) | H19A—C19—H19B | 109.5 |
| O1—C9—C8 | 114.81 (19) | C16—C19—H19C | 109.5 |
| C1—C9—C8 | 120.1 (2) | H19A—C19—H19C | 109.5 |
| O1—C10—C11 | 107.17 (18) | H19B—C19—H19C | 109.5 |
| O1—C10—H10A | 110.3 | HWB—OW—HWA | 104 (3) |
| C11—C10—H10A | 110.3 | | |

| | | | |
|---|---|---|---|
| C9—C1—C2—C3 | 0.0 (4) | C12—N2—C11—O2 | 0.9 (3) |
| C1—C2—C3—C4 | −0.8 (4) | C12—N2—C11—C10 | −177.9 (2) |
| C11—O2—N3—C12 | −0.1 (3) | N3—O2—C11—N2 | −0.5 (3) |
| C2—C3—C4—C5 | −178.5 (2) | N3—O2—C11—C10 | 178.5 (2) |
| C2—C3—C4—C8 | 0.6 (4) | O1—C10—C11—N2 | 5.4 (4) |
| C3—C4—C5—C6 | 179.2 (2) | O1—C10—C11—O2 | −173.34 (19) |
| C8—C4—C5—C6 | 0.1 (4) | O2—N3—C12—N2 | 0.7 (3) |
| C4—C5—C6—C7 | 0.0 (4) | O2—N3—C12—C13 | −177.1 (2) |
| C8—N1—C7—C6 | 0.1 (4) | C11—N2—C12—N3 | −1.0 (3) |
| C5—C6—C7—N1 | −0.1 (4) | C11—N2—C12—C13 | 176.7 (2) |
| C7—N1—C8—C4 | 0.0 (3) | N3—C12—C13—C14 | −162.3 (3) |
| C7—N1—C8—C9 | −179.5 (2) | N2—C12—C13—C14 | 20.1 (4) |
| C5—C4—C8—N1 | −0.1 (3) | N3—C12—C13—C18 | 17.4 (4) |
| C3—C4—C8—N1 | −179.2 (2) | N2—C12—C13—C18 | −160.1 (3) |
| C5—C4—C8—C9 | 179.4 (2) | C18—C13—C14—C15 | −1.8 (4) |
| C3—C4—C8—C9 | 0.3 (3) | C12—C13—C14—C15 | 177.9 (2) |
| C10—O1—C9—C1 | 1.1 (3) | C13—C14—C15—C16 | 0.9 (4) |
| C10—O1—C9—C8 | 179.53 (19) | C14—C15—C16—C17 | 0.4 (4) |
| C2—C1—C9—O1 | 179.3 (2) | C14—C15—C16—C19 | −178.6 (3) |
| C2—C1—C9—C8 | 0.9 (4) | C15—C16—C17—C18 | −0.7 (5) |
| N1—C8—C9—O1 | 0.0 (3) | C19—C16—C17—C18 | 178.2 (3) |
| C4—C8—C9—O1 | −179.54 (19) | C16—C17—C18—C13 | −0.2 (5) |
| N1—C8—C9—C1 | 178.5 (2) | C14—C13—C18—C17 | 1.5 (5) |
| C4—C8—C9—C1 | −1.1 (3) | C12—C13—C18—C17 | −178.2 (3) |
| C9—O1—C10—C11 | 174.34 (18) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O*W*—H*WB*···N2 | 0.91 (3) | 2.09 (3) | 2.980 (3) | 169 (3) |
| O*W*—H*WA*···N1 | 0.94 (3) | 1.91 (3) | 2.830 (3) | 165 (3) |
| C7—H7*A*···O*W*$^{i}$ | 0.93 | 2.51 | 3.272 (3) | 139 |
| C10—H10*A*···O*W*$^{ii}$ | 0.97 | 2.55 | 3.482 (3) | 160 |
| C10—H10*B*···O*W*$^{iii}$ | 0.97 | 2.59 | 3.534 (3) | 164 |

Symmetry codes: (i) −*x*−1, −*y*+1, −*z*+2; (ii) *x*+1, *y*, *z*; (iii) −*x*, −*y*+2, −*z*+2.